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A Gap between Liquid and Crystal of Hard Spheres

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剛体球系の自由エネルギーを評価するために，剛体球同士の重なりを許して，重なりの程度を表すパラメーターを導入し，理想気体と剛体球系の間の内挿を試みた．その結果について報告する．

Hard repulsive particles can describe soft matters. For example, hard spheres, hard ellipsoids of revolution, and so forth, express structures of crystal, liquid, and liquid crystals. They are still new for the development of molecular science.

Potential energy U of the systems of hard repulsive particles is so simple.

$$U = \begin{cases} \infty, & \text{if particles intersect,} \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

To study the singularity of the systems of hard repulsive particles, we consider energy U_h,

$$U_h = h\sigma, \tag{2}$$

where extensive variable σ is degree of intersection, and intensive variable h is the field related to σ.

The U_0 corresponds to the case of the ideal gas. We define σ as U_∞ corresponds the hard repulsive case U. One possible σ is $\sigma = \sum_{j<k} \phi_{jk}$, where

$$\phi_{jk} = \begin{cases} 1, & \text{if j-th and k-th particles intersect,} \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

When we write average of quantity x for U_h as $\langle x \rangle_h$,

$$\langle \sigma \rangle_\infty = 0, \tag{4}$$

in the case of equation (3). For hard spheres, we have

$$\langle \sigma \rangle_0 = \frac{(N-1)N}{V} B_2, \tag{5}$$

where B_2 is the second virial coefficient, N number of particles, and V volume of the system.

We perform constant NVT Monte Carlo (MC) simulation of hard spheres using U_h. When density of the system corresponds to one of liquid phase of U_∞, simulations of various $h's$ indicate continuous change of distribution of σ. When the density corresponds to crystal phase of U_∞, they indicate a discontinuity between crystal and liquid phases.

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